

Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

## Prof. Dr. Frank Noe

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## Četrtek / Thursday 19. 11. 2020, ob / at 13:00

NA DALJAVO / ONLINE WEBEX Povezava/link:

https://ki-si.webex.com/ki-si/j.php?MTID=m02cb04f3240ac9aea00b722473445628

Meeting number: 163 994 0095 Password: kemijski2020

## **Deep Learning for Molecular Physics**

Artificial intelligence (AI), and specifically deep machine learning (ML) methods have a profound impact on industry and information technology. But since recently AI methods are also changing the way we do science. In this talk I will present some of our recent efforts to build machine learning methods that attack fundamental problems in physical and chemical sciences: the sampling problem in physical manybody systems, and the solution of the quantum-chemical electronic Schrödinger equation. Key in making progress in these hard problems with ML is to interrogate the physical system about what the learning problem should be, and to encode physical structures, such as symmetries and conservation laws, into the ML model.

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